Applied Quantum Mechanics: Assignment #1

Due on Thursday, November 5, 2015

Prof. Dr. Erik Koch

Ushnish Sengupta

Problem 1

An electron is in a potential well of 1.2 nm with infinitely high potential barriers on either side. It is in the lowest possible state. What is its energy? What would be the probability of finding the electron between 0.1 and 0.3 nm from one side of the well?

$\psi_n = \sqrt{2/L}\sin(xn\pi/L)$
$E_n = n^2\hbar^2\pi^2/2mL^2$
In the given problem
$L = 1.2\ nm$
$n = 1$
Substituting we get:
$E_1 = 4.1834 \times 10^{-20} J = 0.2611\ eV$ (Ans.)

We know the required probability is given by
$\int_0^{0.3} |\psi^2| dx = \int_0^{0.3} \frac{2}{1.2}\sin^2(x\pi/1.2)dx = 0.08708$ (Ans.)

Problem 2

Consider an electron in a three dimensional box of side lengths L with infinitely high potential walls.

1. Use separation of variables to find the eigenstates and eigenenergies of this three-dimensional box in terms of the eigenstates and eigenenergies of the one-dimensional particle in a box problem.

2. Find an expression for the allowed energies of the electron in this box in terms of the lowest allowed energy E_1^∞ of a particle in a one-dimensional box of width L.

3. Explicitly write down the wavefunctions of the four lowest energy states. Dierent states of the same energy are called degenerate. Which of the states that you have calculated are degenerate?

Problem 2 continued on next page. . .

(1)

Since V is 0 in the box, the time independent equation $H\psi = E\psi$ becomes
$-(\hbar^2/2m)(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}) = E\Psi$
Now using seperation of variables we can write
$\psi = X(x)Y(y)Z(z)$
Substituting the above in the time independent equation and dividing both sides by ψ we get
$-(\hbar^2/2m)(\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} + \frac{1}{Z}\frac{d^2Z}{dz^2}) = E$
Now here we have the sum of three functions of three independent variables! Each of these functions, must therefore, equal a constant. Thus we have the three equations
$\frac{d^2X}{dx^2} + (2m/\hbar^2)E_xX = 0$
$\frac{d^2Y}{dy^2} + (2m/\hbar^2)E_yY = 0$
$\frac{d^2Z}{dz^2} + (2m/\hbar^2)E_zZ = 0$
where $E_x + E_y + E_z = E$
But these are merely 1D particle in a box problems in the X, Y and Z dimensions.
So we can now write
$X(x) = \sqrt{\frac{2}{L}}\sin(xn_x\pi/L_x)\ E_x = \frac{\hbar^2\pi^2n_x^2}{2mL^2}$
$Y(y) = \sqrt{\frac{2}{L}}\sin(yn_y\pi/L_y)\ E_y = \frac{\hbar^2\pi^2n_y^2}{2mL^2}$
$Z(z) = \sqrt{\frac{2}{L}}\sin(zn_z\pi/L_z)\ E_z = \frac{\hbar^2\pi^2n_z^2}{2mL^2}$
From $E_x + E_y + E_z = E$ we can now write
$E_x = \frac{\hbar^2\pi^2(n_x^2+n_y^2+n_z^2)}{2mL^2}$
And from $\psi = X(x)Y(y)Z(z)$ we get
$\psi = (\frac{2}{L})^{\frac{3}{2}}\sin(xn_x\pi/L)\sin(yn_y\pi/L)\sin(zn_z\pi/L)$

(2)

The lowest allowed energy state is evidently where $(n_x, n_y, n_y) = (1, 1, 1)$.
Thus $E_1^\infty = \frac{3\hbar^2\pi^2}{2mL^2}$.
Therefore $E_{(n_x,n_y,n_z)} = \frac{E_1^\infty(n_x^2+n_y^2+n_z^2)}{3}$ (Ans.)

(3)

The lowest energy states are attained when $(n_x, n_y, n_z) = (1, 1, 1), (2, 1, 1), (1, 2, 1), (1, 1, 2)$
The wavefunctions are
$\psi_{(1,1,1)} = (\frac{2}{L})^{\frac{3}{2}}\sin(x\pi/L)\sin(y\pi/L)\sin(z\pi/L)$
$\psi_{(2,1,1)} = (\frac{2}{L})^{\frac{3}{2}}\sin(2x\pi/L)\sin(y\pi/L)\sin(z\pi/L)$
$\psi_{(1,2,1)} = (\frac{2}{L})^{\frac{3}{2}}\sin(x\pi/L)\sin(2y\pi/L)\sin(z\pi/L)$
$\psi_{(1,1,2)} = (\frac{2}{L})^{\frac{3}{2}}\sin(x\pi/L)\sin(y\pi/L)\sin(2z\pi/L)$
Energies are equal for those states for which the sum of squares of the quantum numbers are equal so the states $(2, 1, 1)$, $(1, 2, 1)$ and $(1, 1, 2)$ are degenerate. (Ans.)

Problem 3

Python Code for 1D Quantum Well:

```
import numpy as np
import matplotlib.pyplot as plt

print ("Enter Length of 1D Potential Well in Nanometers:")

lengthxstring = input()
lengthx = float(lengthxstring)

print ("Enter Energy Level")
nstring = input()
n = float(nstring)

x = np.arange(0., lengthx, (lengthx-0)/1000)
psi = np.sqrt(2/lengthx)*np.sin((x)*(n*3.14/lengthx))
plt.plot(x, psi)
plt.ylabel('WAVE FUNCTION')
plt.xlabel('LOCATION')
plt.show()
```

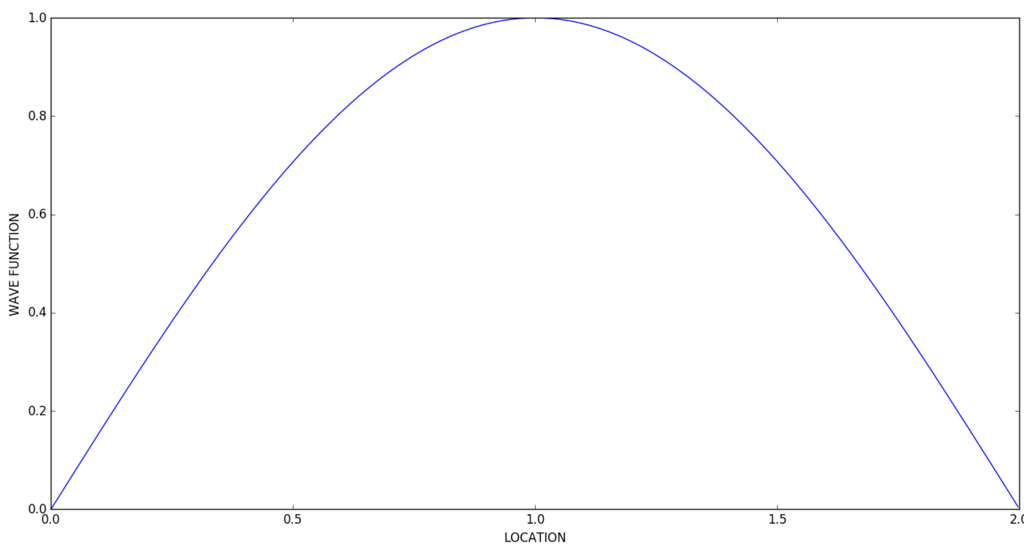

Fig 1: Plot of Time-Independent wave function for $n = 1$

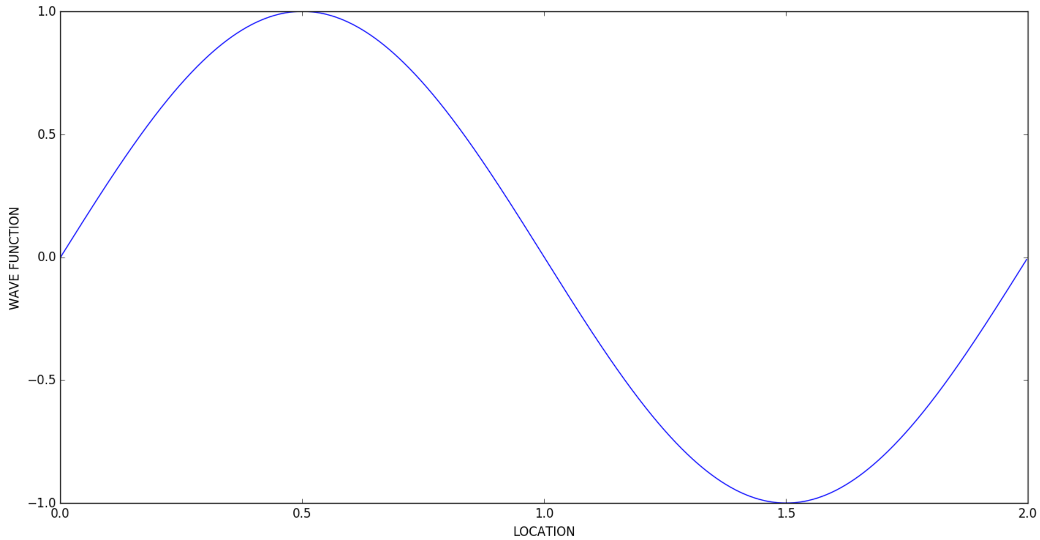

Fig 2: Plot of Time-Independent wave function for $n = 2$

Python Code for 2D Quantum Well:

```
import numpy as np
import matplotlib.pyplot as plt
from matplotlib.mlab import griddata
from mpl_toolkits.mplot3d import Axes3D
from matplotlib import cm
from matplotlib.ticker import LinearLocator, FormatStrFormatter
from pylab import meshgrid,cm,imshow,contour,clabel,colorbar,axis,title,show

print ("Enter X Length of 1D Potential Well in nanometres:")
lengthxstring = input()
lengthx = float(lengthxstring)

print ("Enter Y Length of 1D Potential Well in nanometres:")
lengthystring = input()
lengthy = float(lengthystring)

print ("Enter nx:")
nxstring = input()
nx = float(nxstring)

print ("Enter ny:")
nystring = input()
ny = float(nystring)

x = np.arange(0., lengthx, (lengthx-0)/100)
y = np.arange(0., lengthy, (lengthy-0)/100)
```

```
def psi(x, y):
    return (np.sqrt(2/lengthx)*np.sqrt(2/lengthx)*np.sin((x)*(nx*3.14/lengthx))
    \*np.sin((y)*(ny*3.14/lengthy)))
X1,Y1 = meshgrid(x, y)
Z = psi(X1, Y1)
fig = plt.figure()
ax = fig.gca(projection='3d')
surf = ax.plot_surface(X1, Y1, Z, rstride=1, cstride=1,
                       cmap=cm.RdBu,linewidth=0, antialiased=False)

ax.zaxis.set_major_locator(LinearLocator(10))
ax.zaxis.set_major_formatter(FormatStrFormatter('%.02f'))
ax.set_xlabel('X LOCATION')
ax.set_ylabel('Y LOCATION')
ax.set_zlabel('WAVE FUNCTION')
fig.colorbar(surf, shrink=0.5, aspect=5)

plt.show()
```

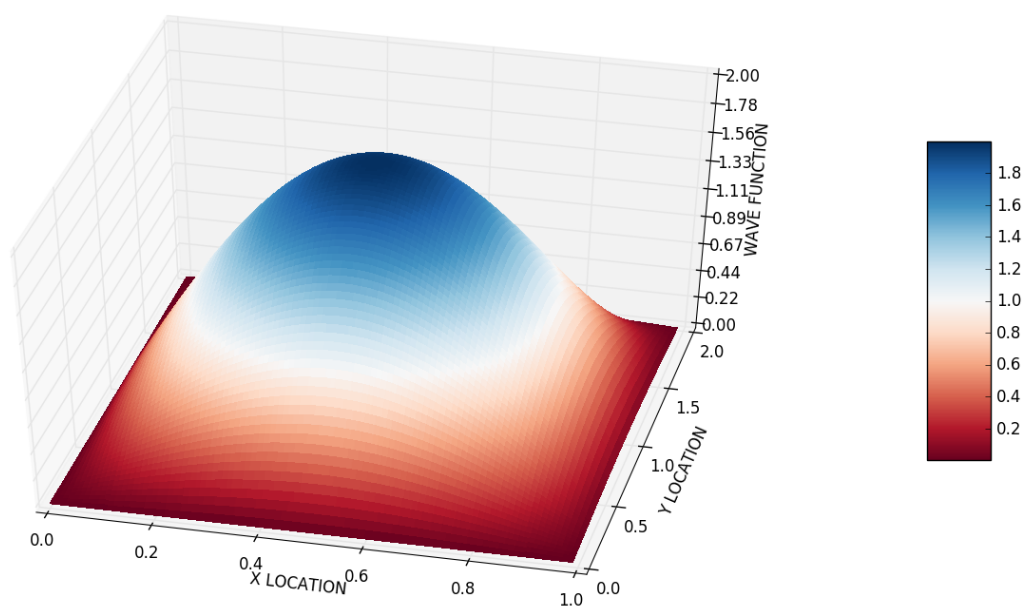

Fig 4: Plot of Time-Independent wave function for $n_x = 1, n_y = 1$

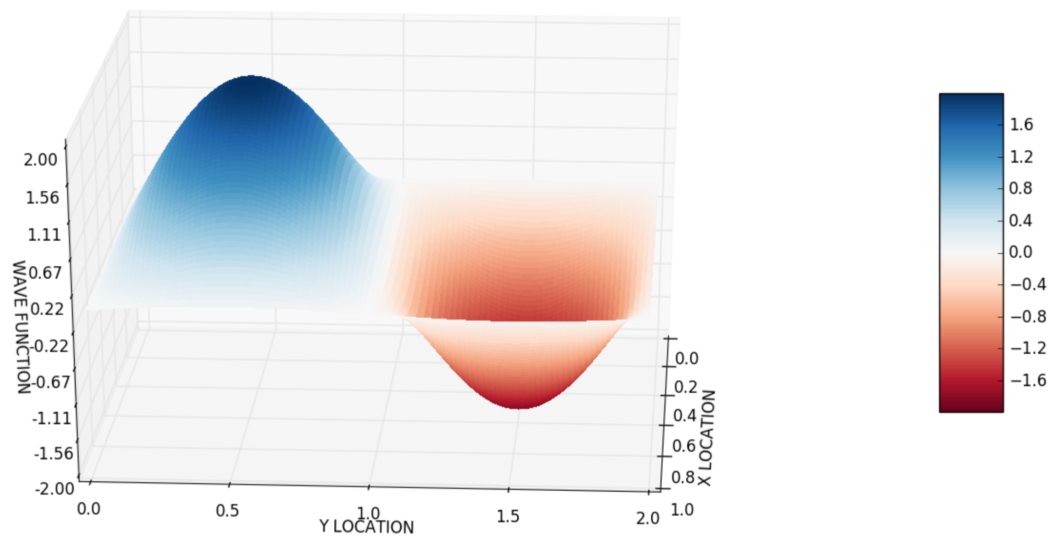

Fig 5: Plot of Time-Independent wave function for $n_x = 1, n_y = 2$

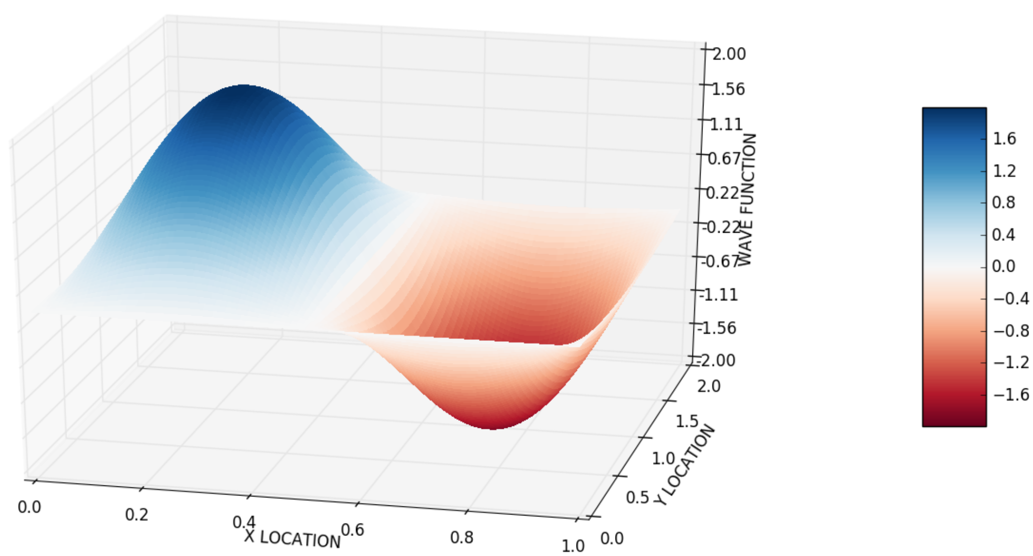

Fig 6: Plot of Time-Independent wave function for $n_x = 2, n_y = 1$